Novel Non-Precious Metals for PEMFC: Catalyst Selection Through Molecular Modeling and Durability Studies (New FY 2004 Project)

Dr. Branko N. Popov (Primary Contact)
Department of Chemical Engineering
Swearingen Engineering Center
University of South Carolina (USC)
Columbia, SC 29208
Phone: (803) 777-7314; Fax: (803) 777-8265; E-mail: popov@engr.sc.edu

DOE Technology Development Manager: Donna Ho
Phone: (202) 586-8000; Fax: (202) 586-9811; E-mail: Donna.Ho@ee.doe.gov

Objectives

- Construct and test membrane electrode assemblies (MEAs) with different non-precious metallic nanoclusters.
- Demonstrate the potential of non-precious metal catalysts to perform at least as well as the conventional Pt catalysts currently in use in MEAs and cost at least 50% less while meeting a target of 0.2 g (Pt loading)/peak kW.
- Optimize the catalyst composition for durability of >2000 hours operation with less than 10% power degradation.
- Perform slab band surface calculation of H_2O and OH adsorption on novel catalysts. Based on this, we will identify promising catalysts and optimize their compositions.

Technical Barriers

This project addresses the following technical barriers from the Fuel Cells section of the Hydrogen, Fuel Cells and Infrastructure Technologies Program Multi-Year R,D&D Plan:

- O. Manufacturing Cost
- P. Durability
- Q. Electrode Performance

Approach

The goal of the proposed work is to construct and test membrane electrode assemblies (MEAs) with different non-precious metallic nanoclusters. The objective is to demonstrate the potential of non-precious metal catalysts to perform at least as well as the conventional Pt catalysts currently in use in MEAs and cost at least 50% less while meeting a target of 0.2 g (Pt loading)/peak kW. Apart from activity, optimization of catalyst composition will be based on durability of >2000 hours operation with less than 10% power degradation. Performance (activity and stability) of the following three different types of metallic nanoclusters will be extensively studied: (i) metal carbon nanoclusters; (ii) non-precious chalcogen compounds and (iii) binary transition metal microcycles. The approach takes advantage of recent accomplishments in USC cathode catalyst development which have drastically reduced the thickness of the catalyst layer and the precious metal content of Pt-based binary catalysts.

Theoretical studies will be conducted to determine the electronic, geometric, and thermodynamic factors that determine catalytic

and electrocatalytic behavior as observed from the experimental characterization. Theoretical studies will comprise a series of high level *ab initio* investigations on representative clusters as well as on extended systems focusing on fundamental interactions relevant to adsorption and reaction processes.

The proposed work is divided into five tasks. The first task is focused on molecular modeling of novel catalysts. The work will include Vienna ab Initio Simulation Program (VSAB) slab band calculation to model surface adsorption of H_2O and O_2 reduction intermediates for the purpose of estimating their reversible potentials of formation. The second task is focused on synthesis of novel catalysts, which will include: (i) synthesis of metal carbon nanoclusters; (ii) synthesis of non-precious chalcogen compounds and (iii) synthesis of binary transition metal microcycles. The third task targets the material characterization of the catalysts. The fourth task focuses on electrochemical characterization, including electrochemical characterization of thin film membrane assemblies and optimization studies of nanostructured electrode/electrolyte interface. The fifth task will optimize the stability of the catalysts. The objective of this task is to evaluate the long-term performance of the composite electrodes. Tafel and linear polarization (LP) technique and conventional three-electrode setup will be used to estimate the corrosion rates of the electrocatalysts in sulfuric acid. To test the long-term performance of the electrocatalyst under real environmental conditions, a single test cell will be used coupled with the test station. The infrared polarization test will be performed as a function of time (300 hours) at constant potential of 0.8 V.

This work will be done in collaboration between University of South Carolina (USC); Case Western Reserve University (CWRU), Cleveland, Ohio; and Northeastern University, Boston, Massachusetts.